STABILITY OF RELATIVISTIC MATTER WITH MAGNETIC FIELDS FOR NUCLEAR CHARGES UP TO THE CRITICAL VALUE

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ABSTRACT. We give a proof of stability of relativistic matter with magnetic fields all the way up to the critical value of the nuclear charge $Z\alpha = 2/\pi$.

1. Introduction

We shall give a proof of the 'stability of relativistic matter' that goes further than previous proofs by permitting the inclusion of magnetic fields for values of the nuclear charge Z all the way up to $Z\alpha=2/\pi$, which is the well known critical value in the absence of a field. (The dimensionless number $\alpha=e^2/\hbar c$ is the 'fine-structure constant' and equals 1/137.036 in nature.) More precisely, we shall show how to modify the earlier proof of Theorem 2 in [LY] so that an arbitrary magnetic field can be included. Reference will freely be made to items in the [LY] paper.

The quantum mechanical Hamiltonian used here and in [LY], as well as the definition of stability of matter, will be given in the next section. For a detailed overview of this topic, we refer to [L1, L2]. For the present we note that stability requires a bound on α in two ways. One is the requirement, for any number of electrons, that $Z\alpha \leq 2/\pi$. In fact, if $Z\alpha > 2/\pi$ the Hamiltonian is not bounded below even for a single electron. The other requirement is a bound on α itself, $\alpha \leq \alpha_c$, even for arbitrarily small Z > 0, which comes into play when the number of particles is sufficiently large. It is known that $\alpha_c \leq 128/15\pi$; see [LY, Thm. 3] and also [DL].

For values of $Z\alpha$ strictly smaller than the critical value $2/\pi$, it has been shown that stability holds with a magnetic field included. This is the content of Theorem 1 in [LY], in which the critical value of α_c goes to zero as $Z\alpha$ approaches $2/\pi$, however. (The result in [LY, Theorem 1] does not explicitly include a magnetic field, but the fact that the proof can easily be modified was noted in [LLoSo].) A similar result, by a different method, was proved in [LLoSi].

The more refined Theorem 2 in [LY] gives stability for the 'natural' value $Z\alpha \leq 2/\pi$ and all $\alpha \leq 1/94$. While the true value of α_c is probably closer to 1, the value 1/94 > 1/137 is sufficient for physics. The problem with the proof of [LY, Theorem 2] is that it does not allow for the inclusion of magnetic fields. Specifically, Theorems

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9–11 have to be substantially modified, and doing so was an open problem for many years. This will be accomplished here at the price of decreasing α_c from 1/94 to 1/133. Fortunately, this is still larger than the physical value 1/137!

In a closely related paper [FLSe] we also show how to achieve a proof of stability for all $Z\alpha \leq 2/\pi$ with an arbitrary magnetic field, but the value of α_c there is very much smaller than the value obtained here. In particular, the physical value of $\alpha=1/137$ is not covered by the result in [FLSe]. The focus of [FLSe] is much broader than 'stability of matter', however. It is concerned with a general connection between Sobolev and Lieb-Thirring type inequalities, and includes as a special case Theorem 4.5 of this paper. The proof of the general result in [FLSe] is much more involved than the one of the special case presented here, and yields a worse bound on the relevant constant.

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2. Definitions and Main Theorem

We consider N electrons of mass $m \geq 0$ with q spin states (q = 2 for real electrons) and K fixed nuclei with (distinct) coordinates $R_1, \ldots, R_K \in \mathbb{R}^3$ and charges $Z_1, \ldots, Z_K > 0$. The electrons interact with an external, spatially dependent magnetic field B(x), which is given in terms of the magnetic vector potential A(x) by B = curl A. A pseudo-relativistic description of the corresponding quantum-mechanical system is given by the Hamiltonian

$$H_{N,K} := \sum_{j=1}^{N} \left(\sqrt{(p_j + A(x_j))^2 + m^2} - m \right) + \alpha V_{N,K}(x_1, \dots, x_N; R_1, \dots, R_k) . \quad (2.1)$$

The Pauli exclusion principle for fermions dictates that $H_{N,K}$ acts on functions in the anti-symmetric N-fold tensor product $\wedge^N L^2(\mathbb{R}^3; \mathbb{C}^q)$. We use units in which $\hbar = c = 1$, $\alpha > 0$ is the fine structure constant, and

$$V_{N,K}(x_1, \dots, x_N; R_1, \dots R_K) := \sum_{1 \le i < j \le N} |x_i - x_j|^{-1} - \sum_{j=1}^N \sum_{k=1}^K Z_k |x_j - R_k|^{-1} + \sum_{1 \le k < l \le K} Z_k Z_l |R_k - R_l|^{-1}.$$
(2.2)

is the Coulomb potential (electron-electron, electron-nuclei, nuclei-nuclei, respectively). In this model there is no interaction of the electron spin with the magnetic field. Note that we absorb the electron charge $\sqrt{\alpha}$ into the vector potential A, i.e., we write A(x) instead of $\sqrt{\alpha}A(x)$ in (2.1). Since A is arbitrary and our bounds are independent of A, this does not affect our results.

Stability of matter means that $H_{N,K}$ is bounded from below by a constant times (N+K), independently of the positions R_k of the nuclei and of A. For a thorough discussion see [L1, L2]. By scaling all spatial coordinates it is easy to see that either $\inf_{R_k,A}(\inf \operatorname{spec} H_{N,K}) = -mN$ or $= -\infty$.

We shall prove the following.

Theorem 2.1 (Stability of relativistic matter with magnetic fields). For $q\alpha \leq 1/66.5$ and $\alpha Z_j \leq 2/\pi$ for all j,

$$H_{N,K} \ge -mN$$

for all N, K, R_1, \ldots, R_K and A.

For electrons q=2 and hence our proof works up to

$$\alpha = \frac{1}{133} > \frac{1}{137}$$
.

The rest of this paper contains the proof of Theorem 2.1, but let us first state an obvious fact.

Corollary 2.2. As a multiplication operator on $\wedge^N L^2(\mathbb{R}^3; \mathbb{C}^q)$,

$$V_{N,K}(x_1, \dots, x_N; R_1, \dots R_K) \ge -\max\{66.5 \, q, \ \pi Z_j/2\} \sum_{j=1}^N |p_j + A(x_j)|$$
 (2.3)

for all A.

This, of course, is just a rewording of Theorem 2.1, but the point is that it provides a lower bound for the Coulomb potential of interacting particles in terms of a one-body operator |p + A(x)|. This operator is dominated by the *nonrelativistic* operator $|p + A(x)|^2$ and, therefore, (2.3) is useful in certain nonrelativistic problems. For example, an inequality of this type was used in [LLoSo] to prove stability of matter with the Pauli operator $|p + A(x)|^2 + \sigma \cdot B(x)$ in place of $|p + A(x)|^2$. It was also used in [LSiSo] to control the no-pair Brown-Ravenhall relativistic model.

An examination of the proof of Theorem 2 in [LY] shows that there are two places that do not permit the inclusion of a magnetic vector potential A. These are Theorem 9 (Localization of kinetic energy – general form) and Theorem 11 (Lower bound to the short-range energy in a ball). Our Theorem 3.1 is precisely the extension of Theorem 9 to the magnetic case. It may be regarded as a diamagnetic inequality on the localization error. It implies that Theorem 10 in [LY] holds also in the magnetic case, without change except for replacing |p| by |p + A|; see Theorem 3.2 below.

A substitute for Theorem 11 in [LY] will be given in Theorem 4.5 below. It is based on the observation that an estimate on eigenvalue sums of a non-magnetic operator with discrete spectrum implies a similar estimate (with a modified constant) for the corresponding magnetic operator. This is not completely obvious, since there is no diamagnetic inequality for *sums* of eigenvalues. (In fact, a conjectured diamagnetic inequality actually fails for fermions on a lattice and leads to the 'flux phase' [L3].) It

is for the different constants in Theorem 11 in [LY] and in our Theorem 4.5 that our bound on α_c become worse than the one in [LY].

As should be clear from the above discussion, our main tool will be a diamagnetic inequality for single functions. The one we use is the diamagnetic inequality for the heat kernel. In the relativistic case it states that for any $A \in L^2_{loc}(\mathbb{R}^3; \mathbb{R}^3)$ and $u \in L^2(\mathbb{R}^3)$ one has

$$\left| \left(\exp(-t|p+A|)u \right)(x) \right| \le \left(\exp(-t|p|)|u| \right)(x), \quad x \in \mathbb{R}^3.$$
 (2.4)

This follows with the help of the subordination formula

$$e^{-|\xi|} = \int_0^\infty e^{-t-|\xi|^2/(4t)} \frac{dt}{\sqrt{\pi t}}$$

from the 'usual' (nonrelativistic) diamagnetic inequality for the semigroup $\exp(-t|p+A|^2)$; see, e.g., [S3]. The heat kernel is not prominent in [LY], and our reformulation of some of the key estimates in [LY] in terms of the heat kernel is the principal novel feature of this paper.

3. Localization of the kinetic energy with magnetic fields

3.1. Relativistic IMS formula. In this subsection we establish the analogue of Theorem 9 in [LY] in the general case $A \neq 0$. First, recall that the IMS formula in the nonrelativistic case says that for any u and A

$$\int_{\mathbb{R}^3} |(p+A)u|^2 dx = \sum_{i=0}^n \int_{\mathbb{R}^3} |(p+A)(\chi_j u)|^2 dx - \int_{\mathbb{R}^3} \sum_{i=0}^n |\nabla \chi_j|^2 |u|^2 dx$$

whenever χ_j are real functions with $\sum_{j=1}^n \chi_j^2 \equiv 1$. In this case the localization error $\sum_{j=0}^n |\nabla \chi_j|^2$ is local and independent of A. The analogue in the relativistic case is the following special case of [FLSe, Lemma B.1]. For the sake of completeness, we include its proof here.

Theorem 3.1 (Localization of kinetic energy – general form). Let $A \in L^2_{loc}(\mathbb{R}^3; \mathbb{R}^3)$. If χ_0, \ldots, χ_n are real Lipschitz continuous functions on \mathbb{R}^3 satisfying $\sum_{j=0}^n \chi_j^2 \equiv 1$, then one has

$$(u, |p+A|u) = \sum_{j=0}^{n} (\chi_j u, |p+A|\chi_j u) - (u, L_A u).$$
(3.1)

Here L_A is a bounded operator with integral kernel

$$L_A(x,y) := k_A(x,y) \sum_{j=0}^n (\chi_j(x) - \chi_j(y))^2,$$

where $k_A(x,y) := \lim_{t \uparrow 0} t^{-1} \exp(-t|p+A|)(x,y)$ for a.e. $x,y \in \mathbb{R}^3$ and

$$|k_A(x,y)| \le \frac{1}{2\pi^2 |x-y|^4}. \tag{3.2}$$

Note that (3.2) says that

$$|L_A(x,y)| \le L(x,y) := \frac{1}{2\pi^2 |x-y|^4} \sum_{j=0}^n (\chi_j(x) - \chi_j(y))^2.$$
 (3.3)

Here, L(x, y) is the same as in [LY, Eq. (3.7)]. Therefore, (3.2) is a diamagnetic inequality for the localization error.

Proof. We write $k_A(x,y,t) := \exp(-t|p+A|)(x,y)$ for the heat kernel and find

$$\sum_{j=0}^{n} (\chi_j u, (1 - \exp(-t|p + A|))\chi_j u) = (u, (1 - \exp(-t|p + A|))u)$$

$$+ \frac{1}{2} \sum_{j=0}^{n} \iint k_{A}(x, y, t) (\chi_{j}(x) - \chi_{j}(y))^{2} \overline{u(x)} u(y) dx dy.$$

(This is proved simply by writing out both sides in terms of $k_A(x, y, t)$ and using $\sum \chi_j^2 \equiv 1$.) Now we divide by t and let $t \to 0$. The left side converges to $\sum_{j=0}^n (\chi_j u, |p+A|\chi_j u)$. Similarly, the first term on the right side divided by t converges to (u, |p+A|u). Hence the last term divided by t converges to some limit $(u, L_A u)$. The diamagnetic inequality (2.4) says that

$$|k_A(x,y,t)| \le \exp(-t|p|)(x,y) = \frac{t}{\pi^2 (|x-y|^2 + t^2)^2}$$

(see [LLo, Eq. 7.11(9)]). This implies, in particular, that L_A is a bounded operator. Now it is easy to check that L_A is an integral operator and that the absolute value of its kernel is bounded pointwise by the one of L in (3.3).

3.2. Localization of the kinetic energy. In this subsection we will bound the localization error L_A by a potential energy correction and an additive constant. This is the extension of Theorem 10 in [LY] to the case $A \neq 0$. It is important that both error terms in our bound can be chosen independently of A.

First we need to introduce some notation. We write

$$\mathcal{B}_R := \{x : |x| < R\}$$

for the ball of radius R and $\chi_{\mathcal{B}_R}$ for its characteristic function. If R=1, we omit the index in the notation. We fix a constant $0 < \sigma < 1$ and Lipschitz continuous functions χ_0, χ_1 with $\chi_0^2 + \chi_1^2 \equiv 1$ such that supp $\chi_1 \subset \overline{\mathcal{B}}_{1-\sigma}$. With these we define L as in (3.3) with n=1. We decompose L in a short-range part L^0 and a long-range part L^1 given by the kernels

$$L^{1}(x,y) := L(x,y)\chi_{\mathcal{B}}(x)\chi_{\mathcal{B}}(y)\chi_{\mathcal{B}_{\sigma}}(x-y), \qquad L^{0}(x,y) := L(x,y) - L^{1}(x,y).$$
(3.4)

Define

$$\Omega := \frac{1}{2} \operatorname{Tr} \left(L^0 \right)^2 \tag{3.5}$$

and, for an arbitrary positive function h on \mathcal{B} ,

$$\theta(x) := h^{-1}(x) \int_{\mathcal{B}} L^1(x,y) h(y) \, dy = h^{-1}(x) \chi_{\mathcal{B}}(x) \int_{|y| < 1, \, |x-y| < \sigma} L(x,y) h(y) \, dy \, .$$

Finally, for $\varepsilon > 0$ we define the function

$$U_{\varepsilon}^* := \varepsilon \chi_{\mathcal{B}_{1-\sigma}} + \theta \tag{3.6}$$

and note that U_{ε}^* is supported in $\overline{\mathcal{B}}$.

Theorem 3.2 (Localization of kinetic energy – explicit bound in the one-center case). For any $\varepsilon > 0$ and any non-negative trace-class operator γ one has

$$\operatorname{Tr} \gamma |p + A| \ge \sum_{j=0}^{1} \operatorname{Tr} \chi_{j} \gamma \chi_{j} (|p + A| - U_{\varepsilon}^{*}) - \varepsilon^{-1} \Omega \|\gamma\|.$$
 (3.7)

For A=0 this is exactly Theorem 10 in [LY]. As explained there, U_{ε}^{*} is a potential energy correction with only slightly larger support than χ_{1} . The last term in (3.7) is due to the long range nature of |p+A|. It depends on γ through its norm $||\gamma||$ but not through its trace. We emphasize again that both error terms in the inequality (3.7) are independent of A.

Proof. The localization formula (3.1) yields

$$\operatorname{Tr} \gamma |p+A| = \sum_{j=0}^{1} \operatorname{Tr} \chi_{j} \gamma \chi_{j} |p+A| - \operatorname{Tr} \gamma L_{A},$$

so we only have to find an upper bound for $\operatorname{Tr} \gamma L_A$. We decompose $L_A = L_A^0 + L_A^1$ in the manner of (3.4) and, following the proof of Theorem 10 in [LY] word by word, we obtain

$$\operatorname{Tr} \gamma L_A^0 \leq \varepsilon \operatorname{Tr} \gamma \chi_{\mathcal{B}_{1-\sigma}} + (2\varepsilon)^{-1} \|\gamma\| \operatorname{Tr} (L_A^0)^2, \quad \operatorname{Tr} \gamma L_A^1 \leq \operatorname{Tr} \gamma \theta_A.$$

Here $\theta_A(x) := 0$ if $x \notin \mathcal{B}$ and, if $x \in \mathcal{B}$,

$$\theta_A(x) := h^{-1}(x) \int_{\mathcal{B}} |L_A^1(x,y)| h(y) \, dy.$$

The estimate $|L_A(x,y)| \leq L(x,y)$ from Theorem 3.1 implies that $\text{Tr}(L_A^0)^2 \leq 2\Omega$ and that $\theta_A \leq \theta$. This leads to the stated lower bound.

4. Bounds on eigenvalues in balls

So far we have considered |p + A| and its heat kernel. Now we address $|p + A| - 2/(\pi|x|)$ and its heat kernel. First of all, let us recall Kato's inequality [Ka, Eq. (V.5.33)]

$$(u, |p|u) \ge (2/\pi)(u, |x|^{-1}u).$$
 (4.1)

(See also [H, W, KPS].)

Now let $\Gamma \subset \mathbb{R}^3$ be an open set (we shall be interested in the case where Γ is a ball) and consider the quadratic form given by $Q_{\Gamma}(u) = (u, (|p| - 2/\pi |x|)u)$, restricted to those functions $u \in L^2(\mathbb{R}^3)$ that satisfy u = 0 on Γ^c , the complement of Γ . Of course, we also require u to be in the quadratic form domain of $|p| - 2/\pi |x|$. The quadratic form Q_{Γ} is non-negative by (4.1) and it is closed (because the form $|p| - 2/\pi |x|$ is closed on $L^2(\mathbb{R}^3)$ and limits of functions that are zero on Γ^c are zero on Γ^c). From this it follows that there is a self-adjoint operator H_{Γ} on some domain in $L^2(\Gamma)$ such that $Q_{\Gamma}(u) = (u, H_{\Gamma}u)$. With this operator, we can define the 'heat kernel' $\exp(-tH_{\Gamma})$ on $L^2(\Gamma)$ and its trace. (The fact that the trace is finite when the volume of Γ is finite follows from subsequent considerations.)

Similarly, for a magnetic vector potential $A \in L^2_{loc}(\mathbb{R}^3; \mathbb{R}^3)$, we define the operator H^A_{Γ} in $L_2(\Gamma)$ using the quadratic form $(u, (|p+A|-2/\pi|x|)u)$. Note that (2.4) implies that

$$(u, |p+A|u) \ge (|u|, |p||u|).$$
 (4.2)

This, together with (4.1), shows that $(u, (|p+A|-2/\pi|x|)u)$ is non-negative.

Lemma 4.1 (Heat kernel diamagnetic inequality). Let $\Gamma \subset \mathbb{R}^3$ and let $A \in L^2_{loc}(\mathbb{R}^3; \mathbb{R}^3)$. Then, for any t > 0,

$$\operatorname{Tr}_{L^2(\Gamma)} \exp\left(-tH_{\Gamma}^A\right) \le \operatorname{Tr}_{L^2(\Gamma)} \exp\left(-tH_{\Gamma}\right)$$
 (4.3)

Proof. For n = 0, 1, 2, ... let $h_n := |p| - 2/(\pi|x|) + n\chi_{\Gamma^c}$ in $L^2(\mathbb{R}^3)$, where χ_{Γ^c} denotes the characteristic function of the complement of Γ . Similarly, let $h_n^A := |p + A| - 2/(\pi|x|) + n\chi_{\Gamma^c}$. The diamagnetic inequality (2.4) and standard approximation arguments using Trotter's product formula imply that, for any $u \in L^2(\mathbb{R}^3)$,

$$\left|\left(\exp(-th_n^A)u\right)(x)\right| \le \left(\exp(-th_n)|u|\right)(x).$$

(See [FLSe, Section 6.2] for details of the argument.)

By the monotone convergence theorem [S1, Thm. 4.1], $\exp(-th_n)$ converges strongly to $\exp(-tH_{\Gamma})$ on the subspace $L^2(\Gamma)$, and similarly for h_n^A . It follows that, for any $u \in L^2(\Gamma)$,

$$\left| \left(\exp(-tH_{\Gamma}^A)u \right)(x) \right| \le \left(\exp(-tH_{\Gamma})|u| \right)(x).$$

Theorem 2.13 in [S3] yields the inequality $\|\exp(-tH_{\Gamma}^A)\|_2 \leq \|\exp(-tH_{\Gamma})\|_2$ for the Hilbert-Schmidt norm, and hence $\|\exp(-2tH_{\Gamma}^A)\|_1 \leq \|\exp(-2tH_{\Gamma})\|_1$ for the trace norm by the semigroup property. This holds for all t > 0, and hence proves (4.3).

We use the notation $(x)_{-} = \max\{0, -x\}$ for the negative part of $x \in \mathbb{R}$ in the following.

Lemma 4.2. Assume that there is constant M > 0 such that

$$\operatorname{Tr}_{L^{2}(\Gamma)}(H_{\Gamma} - \Lambda)_{-} \leq M\Lambda^{4} \tag{4.4}$$

for all $\Lambda \geq 0$. Then

$$\operatorname{Tr}_{L^{2}(\Gamma)}\left(H_{\Gamma}^{A}-\Lambda\right)_{-} \leq \frac{6e^{3}}{4^{3}}M\Lambda^{4} \tag{4.5}$$

for all $\Lambda \geq 0$.

We note the numerical factor in (4.5) equals $6(e/4)^3 \approx 1.883$. This factor is the price we have to pay, using our methods, to include an arbitrary magnetic field. It is the reason of the decrease of α_c from 1/94 to 1/133.

Proof. Since $(x)_{-} \leq e^{-x-1}$, we have

$$\operatorname{Tr}_{L^2(\Gamma)} \left(H_{\Gamma}^A - \Lambda \right)_- \le \frac{e^{t\Lambda}}{te} \operatorname{Tr}_{L^2(\Gamma)} \exp \left(-t H_{\Gamma}^A \right)$$

for any t > 0. Using the diamagnetic inequality (4.3),

$$\operatorname{Tr}_{L^2(\Gamma)} \exp\left(-tH_{\Gamma}^A\right) \leq \operatorname{Tr}_{L^2(\Gamma)} \exp\left(-tH_{\Gamma}\right)$$
.

Moreover, integrating by parts twice, $e^{-tx} = t^2 \int_0^\infty e^{-t\lambda} (x-\lambda)_- d\lambda$, and hence

$$\operatorname{Tr}_{L^{2}(\Gamma)} \exp\left(-tH_{\Gamma}\right) = t^{2} \int_{0}^{\infty} e^{-t\lambda} \operatorname{Tr}_{L^{2}(\Gamma)} \left(H_{\Gamma} - \lambda\right)_{-} d\lambda.$$

Using the assumption (4.4), we thus obtain

$$\operatorname{Tr}_{L^2(\Gamma)} \left(H_{\Gamma}^A - \Lambda \right)_- \leq \frac{t e^{t\Lambda}}{e} M \int_0^\infty e^{-t\lambda} \lambda^4 d\lambda = 24 \frac{e^{t\Lambda}}{t^4 e} M.$$

To minimize the right side, the optimal choice of t is $t = 4/\Lambda$. This yields (4.5).

In [LY, Thm. 11] it is shown that (4.4) holds for $\Gamma = \mathcal{B}_R$ a ball of radius R centered at the origin. More precisely, the following proposition holds.

Proposition 4.3. For any R > 0 and $\Lambda \ge 0$,

$$\operatorname{Tr}_{L^2(\mathcal{B}_R)} (H_{\mathcal{B}_R} - \Lambda)_- \le 4.4827 R^3 \Lambda^4.$$

Proposition 4.3 follows from Theorem 11 in [LY] by choosing χ to be the characteristic function of the ball \mathcal{B}_R , q=1 and γ to be the projection onto the negative spectral subspace of $H_{\mathcal{B}_R} - \Lambda$.

Remark 4.4. It is illustrative to compare Proposition 4.3 with the Berezin-Li-Yau type bound

$$\operatorname{Tr}_{L^{2}(\Gamma)}(|p|_{\Gamma} - \Lambda)_{-} \le \frac{1}{(2\pi)^{3}} \int_{\mathbb{R}^{3}} \int_{\Gamma} (|\xi| - \Lambda)_{-} dx d\xi = \frac{1}{24\pi^{2}} \Lambda^{4} |\Gamma|.$$
 (4.6)

(This can be proved in the same way as [LLo, Thm. 12.3].) The right side of (4.6) is the semi-classical phase-space integral. The operator $|p|_{\Gamma}$ is defined as H_{Γ} above, but without the Hardy-term $2/(\pi|x|)$. If the Hardy term were added, the phase-space integral would diverge (provided Γ contains the origin), but Proposition 4.3 says that a bound of the form (4.6) still holds. (An examination of the proof in [LY] shows that Proposition 4.3 actually holds for any open set Γ of finite measure.)

Combining Lemma 4.2 and Proposition 4.3 we obtain the following theorem, which replaces [LY, Thm. 11] in the magnetic case.

Theorem 4.5 (Lower bound on the short-range energy in a ball). Let C>0 and R>0 and let

$$H_{CR}^A:=|p+A|-\frac{2}{\pi|x|}-\frac{C}{R}$$

be defined on $L^2(\mathbb{R}^3)$ as a quadratic form. Let $0 \le \gamma \le q$ be a density matrix (i.e., a positive trace-class operator) and let χ by any bounded function with support in \mathcal{B}_R . Then

$$\operatorname{Tr} \overline{\chi} \gamma \chi H_{CR}^A \ge -8.4411 \frac{qC^4}{R} \|\chi\|_{\infty}^2.$$
 (4.7)

As compared with [LY, Thm. 11], the constant has been multiplied by $6(e/4)^3$, and $\|\chi\|_{\infty}^2$ appears instead of $|\mathcal{B}_R|^{-1}\|\chi\|_2^2$.

Proof. Note that

$$\operatorname{Tr} \overline{\chi} \gamma \chi H_{CR}^A = \operatorname{Tr} \overline{\chi} \gamma \chi \left(H_{\mathcal{B}_R}^A - C/R \right) \ge -\| \overline{\chi} \gamma \chi \|_{\infty} \operatorname{Tr}_{L^2(\mathcal{B}_R)} (H_{\mathcal{B}_R}^A - C/R)_{-}.$$

The assertion follows from Lemma 4.2 and Proposition 4.3, observing that $\|\overline{\chi}\gamma\chi\|_{\infty} \leq q\|\chi\|_{\infty}^2$.

5. Proof of Theorem 2.1

We assume that the reader is familiar with the proof of Theorem 2 in [LY]. We shall only emphasize changes in their argument. The main idea is to replace Theorems 10 and 11 in [LY] by our Theorems 3.2 and 4.5, respectively.

There are some immediate simplifications. First, in view of the simple inequality $\sqrt{|p|^2 + m^2} \ge |p|$ it is enough to prove the Theorem 2.1 for m = 0. Moreover, by the convexity argument of [DL] it suffices to treat the case $Z_1 = \ldots = Z_K =: z$ and $\alpha z = 2/\pi$. So henceforth we assume m = 0, $Z_1 = \ldots = Z_K = z$ and $\alpha z = 2/\pi$.

Let $D_k := \min\{|R_k - R_l| : l \neq k\}$ and define the Voronoi cell

$$\Gamma_k := \{ x \in \mathbb{R}^3 : |x - R_k| < |x - R_l| \text{ for all } l \neq k \}.$$

Fix $0 < \lambda < 1$ and define a function W := G + F in each Voronoi cell by

$$G(x) := z|x - R_k|^{-1}, \qquad F(x) := D_k^{-1}\tilde{F}(|x - R_k|/D_k), \qquad x \in \Gamma_k,$$

where

$$\tilde{F}(t) := \begin{cases} 2^{-1}(1-t^2)^{-1} & \text{if } t \leq \lambda, \\ (\sqrt{2z} + \frac{1}{2})t^{-1} & \text{if } t > \lambda. \end{cases}$$

By the electrostatic inequality in [LY, Sect. III, Step A] our Theorem 2.1 will follow if we can prove that

$$\operatorname{Tr} \gamma(|p+A| - \alpha W) \ge -\frac{z^2 \alpha}{8} \sum_{k=1}^{K} D_k^{-1}$$
 (5.1)

for some $0 < \lambda < 1$ and all density matrices γ with $0 \le \gamma \le q$). Note that (5.1) is an inequality for a *one-particle* operator.

For fixed $0 < \sigma < 1/3$ we choose χ , h as in (3.22), (3.24) in [LY]. Note that supp $\chi \subset \overline{\mathcal{B}_{1-\sigma}}$. Let

$$\chi_k(x) := \chi(|x - R_k|/D_k), \qquad h_k(x) := h(|x - R_k|/D_k).$$

After scaling and translation, Proposition 3.2 yields that for any $0 \le \gamma \le q$

$$\operatorname{Tr} \gamma(|p+A| - \alpha W) \ge \operatorname{Tr} \chi_1 \gamma \chi_1(|p+A| - U_{1,\varepsilon}^* - \alpha W) + \operatorname{Tr} (1 - \chi_1^2)^{1/2} \gamma (1 - \chi_1^2)^{1/2} (|p+A| - U_{1,\varepsilon}^* - \alpha W) - \varepsilon^{-1} q \Omega / D_1.$$
 (5.2)

Here, $U_{1,\varepsilon}^*(x) := D_1^{-1}U_{\varepsilon}^*((x-R_1)/D_1)$ and Ω , U_{ε}^* were defined in (3.5), (3.6). (Note that our Ω is denoted by Ω_1 in [LY]). Recall that U_{ε}^* and Ω are independent of A.

We turn to the first term on the right side of (5.2). Let C be a constant such that

$$C \ge (1 - \sigma) \left(\alpha \tilde{F}(|x|) + U_{\varepsilon}^*(x) \right) \quad \text{for } |x| \le 1 - \sigma.$$
 (5.3)

Note that χ_1 is supported on a ball of radius $(1 - \sigma)D_1$ centered at R_1 . Hence $\alpha W(x) = (2/\pi)|x - R_1|^{-1} + D_1^{-1}\tilde{F}(|x - R_1|/D_1)$ on the support of χ_1 and we can apply Theorem 4.5 to obtain the lower bound

$$\operatorname{Tr} \chi_{1} \gamma \chi_{1}(|D - A| - U_{1,\varepsilon}^{*} - \alpha W) \geq \operatorname{Tr} \chi_{1} \gamma \chi_{1} \left(|p + A| - \frac{2}{\pi |x - R_{1}|} - \frac{C}{(1 - \sigma)D_{1}} \right)$$

$$\geq -8.4411 \frac{qC^{4}}{(1 - \sigma)D_{1}}.$$
(5.4)

We used also that $|\chi_1| \leq 1$. Inserting (5.4) into (5.2) we find

$$\operatorname{Tr} \gamma(|p+A| - \alpha W) \ge -qD_1^{-1}\tilde{A} + \operatorname{Tr}(1-\chi_1^2)^{1/2}\gamma(1-\chi_1^2)^{1/2}(|p+A| - U_{1,\varepsilon}^* - \alpha W)$$

with

$$\tilde{A} := \frac{\Omega}{\varepsilon} + 8.4411 \frac{C^4}{(1-\sigma)}.$$

This estimate is exactly of the form (3.26) in [LY], except for the value of the constant in \tilde{A} (which is called A in [LY]). Starting from there one can continue along the lines of their proof. We need only note that in order to bound the last term in (3.29) in [LY] one uses the Daubechies inequality [D], which holds with the same constant in the presence of a magnetic field. (This is explained, for instance, in [LLoSi, Sect. 5].) We conclude that stability holds as long as

$$\alpha q(\tilde{A} + J) \le \frac{1}{2\pi^2},\tag{5.5}$$

where, as in [LY, Eq. (3.31)],

$$J := 0.0258 \int_{|x| \ge 1 - 3\sigma} \left[\frac{2}{\pi |x|} + \alpha \tilde{F}(|x|) + U_{\varepsilon}^{*}(x) \right]^{4} dx.$$

This completes our proof of Theorem 2.1, except for our bound on the critical α , which we justify now.

As in [LY], we choose $\sigma = 0.3$, $\varepsilon = 0.2077$ and $\lambda = 0.97$. Our goal is to prove stability when $q\alpha \le 1/66.5$. We may assume $\alpha < 1/47$, which is the assumption used in [LY]. Hence we can use the estimate $J \le 1.64$ from [LY, Eq. (3.40)].

To bound \tilde{A} , note that $\varepsilon^{-1}\Omega=0.5571$ as in [LY, Eq. (3.30)]. It remains to choose an appropriate C satisfying (5.3). For $|x| \leq 0.7$ we have $|\tilde{F}(|x|)| \leq 1/1.02$. Moreover, for U_{ε}^* we use the same estimate as in [LY], namely $U_{\varepsilon}^*(x) \leq 0.2077 + 0.5751 = 0.7828$. Using $\alpha \leq 1/(66.5 \, q) \leq 1/66.5$, (5.3) therefore holds with

$$0.7(1/(66.5 \cdot 1.02) + 0.7828) < 0.5583 =: C.$$

This leads to a value of $\tilde{A} = 1.7287$. Hence (5.5) holds for $q\alpha \leq 1/66.5$.

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